

Pentafluoropropionic acid
422-64-0 | DTXSID8059970

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 4.95 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.91e-01

Confidence level: 2.83e-01

Nearest Neighbors from the Training Set

| | | |
|--|--|---|
| <div>Image not found</div> <div>1-Butanol, 2,2,3,3,4,4,4-heptafluoro-</div> <div>Measured: 6.37</div> <div>Predicted: 42.6</div> | <div>Image not found</div> <div>2-Methyl-2-butanol</div> <div>Measured: 110</div> <div>Predicted: 9.41</div> | <div>Image not found</div> <div>Fenamiphos</div> <div>Measured: 3.00e-04</div> <div>Predicted: 1.06e-06</div> |
| <div>Image not found</div> <div>1-Decene</div> <div>Measured: 159</div> <div>Predicted: 1.31</div> | <div>Image not found</div> <div>Ethane, 1,1-dichloro-1,2,2,2-tetrafluoro-</div> <div>Measured: 33.1</div> <div>Predicted: 2170</div> | |